

# Diffusion and ballistic transport in clean one-dimensional conductors

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(Dated: June 10, 2009)

Diffusion and ballistic transport are normally thought to be mutually exclusive phenomena. The reason is that the notion of diffusion entails inelastic scattering processes which typically lead to current relaxation. While diffusive transport is the rule in generic many-body systems, ballistic transport can be protected in integrable one-dimensional (1D) systems by nontrivial conservation laws. The large diffusive response seen experimentally in nearly ideal realizations of the  $S = 1/2$  1D Heisenberg model is therefore puzzling. Here, we show that diffusion is, in fact, universally present in interacting 1D systems subject to a periodic lattice potential and question the conjecture that integrability necessarily leads to ballistic transport. Furthermore, we demonstrate that even at high temperatures current decay can be governed by anomalously large time scales, posing a serious challenge for numerical studies.

## I. INTRODUCTION

For a generic metal at sufficiently high temperatures, electric transport is expected to be scattering limited. In  $d$  spatial dimensions, the signature of diffusive motion is the characteristic long-time decay of the autocorrelation function  $\langle n_{\mathbf{r}}(t)n_{\mathbf{r}}(0) \rangle \sim t^{-d/2}$ . Here,  $n_{\mathbf{r}}$  represents the density of a globally conserved quantity  $\sum_{\mathbf{r}} n_{\mathbf{r}}$ . In very clean metals, however, transport can be a subtle issue because constants of motion of the system may prevent currents from decaying completely, leading to ideal (*ballistic*) transport. An important role in our understanding of strongly correlated electrons is played by *integrable* quantum models. Since these models possess an infinite number of conserved quantities, one might expect ballistic transport to be the rule rather than the exception.<sup>1</sup> Whether or not diffusive behavior is possible at all in such systems is indeed an intensely studied<sup>1-13</sup> but still open question. The unusual dynamics of systems close to an integrable point have been investigated by experiments on ultracold gases in 1D geometries,<sup>14</sup> and is related to the question whether these systems thermalize through unitary evolution.<sup>15</sup>

In the thermodynamic limit, ballistic transport can be defined from the condition that the current-current correlation function  $\langle \mathcal{J}(t)\mathcal{J}(0) \rangle$ , where  $\mathcal{J}$  is the spatial integral of the current density operator and the brackets denote thermal average, does not decay to zero at large times. This happens, for example, in a free electron gas, where  $\mathcal{J}$  is proportional to the momentum operator and therefore conserved in a translationally invariant system.<sup>13</sup> The dc conductivity is then infinite. By contrast, real metals are expected to exhibit diffusive transport (not necessarily connected with diffusion in the autocorrelation function), meaning that any induced current decays to zero. The conductivity is finite and limited by the strongest relaxation process (Matthiessen's rule). A third case is realized in systems where the current operator itself is not conserved but a conserved quantity

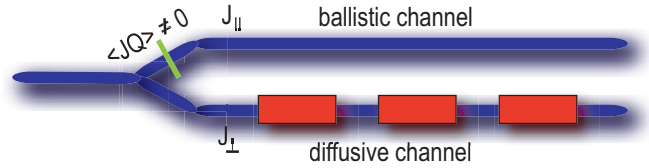


FIG. 1: In a diffusive channel, the conductivity is limited by the dominant of the various scattering processes pictured as a serial arrangement of resistors. If part of the current is, however, protected by a conservation law, a parallel ballistic channel for charge transport is opened.

$Q$  exists which has finite overlap with  $\mathcal{J}$ . We can then write  $\mathcal{J} = \mathcal{J}_{\parallel} + \mathcal{J}_{\perp}$ , with  $\mathcal{J}_{\parallel} = (\langle \mathcal{J}Q \rangle / \langle Q^2 \rangle)Q$  being the part which cannot decay,<sup>9</sup> leading to parallel diffusive and ballistic channels as indicated in Fig. 1. This idea can be generalized to a set of orthogonal conserved quantities  $Q_n$ ,  $\langle Q_n Q_m \rangle = \langle Q_n^2 \rangle \delta_{n,m}$ , and leads to Mazur's inequality<sup>6,16</sup>

$$D = \frac{1}{2LT} \lim_{t \rightarrow \infty} \langle \mathcal{J}(t)\mathcal{J}(0) \rangle \geq \frac{1}{2LT} \sum_n \frac{\langle \mathcal{J}Q_n \rangle^2}{\langle Q_n^2 \rangle}. \quad (1)$$

Here,  $L$  is the system size and  $T$  the temperature. The *Drude weight*  $D$  measures the weight of the delta-function peak in the real part of the optical conductivity at zero frequency,  $\sigma'(\omega) = 2\pi D \delta(\omega) + \sigma_{reg}(\omega)$ . In principle, both  $D$  and  $\sigma_{reg}(\omega = 0)$  can be nonzero.<sup>2</sup> Weak breaking of the conservation laws renders the conductivity finite, but in this case the channel with the smallest decay rate sets a lower bound for the conductivity.<sup>9</sup>

It is important to note that the rhs of equation (1) can vanish even if an infinite number of conserved quantities exists, as we will discuss in the following example. Consider the integrable model of *spinless* fermions (XXZ

model)

$$H = J \sum_{l=1}^N \left[ -\frac{1}{2} \left( c_l^\dagger c_{l+1} + h.c. \right) + \Delta \left( n_l - \frac{1}{2} \right) \left( n_{l+1} - \frac{1}{2} \right) \right]. \quad (2)$$

Here  $N$  is the number of sites,  $J$  the hopping amplitude,  $c_l$  annihilates a fermion at site  $l$ , and  $\Delta$  is the interaction strength. This model is equivalent to the anisotropic spin-1/2 chain and is exactly solvable by Bethe ansatz (BA).<sup>17</sup> At half-filling,  $\langle n_l \rangle = 1/2$ , the excitation spectrum is gapless for  $|\Delta| \leq 1$  and gapped for  $|\Delta| > 1$ . The current operator is  $\mathcal{J} = \sum_l j_l$ , with  $j_l = -iJ(c_l^\dagger c_{l+1} - c_{l+1}^\dagger c_l)/2$  as follows from a discretized continuity equation.

The transport properties of the XXZ model have been studied for many years.<sup>1-13</sup> At zero temperature, the Drude weight can be calculated by BA<sup>18</sup> and is found to be finite in the gapless and zero in the gapped regime. Mazur's inequality can be used to show that  $D(T) \neq 0$  away from half-filling at arbitrary temperatures.<sup>6</sup> Remarkably, at half-filling the Mazur bound for the Drude weight obtained from *all local* conserved quantities vanishes identically due to particle-hole symmetry. Since this is only a lower bound, it does not imply that  $D$  itself vanishes. However, one can argue<sup>19</sup> that in the gapped regime  $D$  should remain zero at finite temperatures. The main open question is whether the Drude weight is finite at finite temperatures in the half-filled gapless case. Since equation (1) is actually an equality if all conserved quantities are included,<sup>20</sup> a nonzero  $D$  at half-filling requires the existence of a *nonlocal* conservation law.<sup>9</sup>  $D(T > 0) \neq 0$  at half-filling has been found in two independent BA calculations.<sup>4,10</sup> However, these results disagree and they both violate exact relations for  $D(T)$  at high temperatures.<sup>10</sup> Further evidence for  $D(T > 0) \neq 0$  stems from exact diagonalization<sup>7-9</sup> and Quantum Monte Carlo (QMC).<sup>5,21</sup> We will discuss these numerical works in relation to our own results in section III.

Evidence for diffusion in the spin-spin autocorrelation function at high temperatures has been sought via exact diagonalization,<sup>11</sup> QMC<sup>22</sup> and density matrix renormalization group (DMRG).<sup>12,23</sup> The results at infinite temperature seemed consistent with an algebraic decay  $\langle S_l^z(t) S_l^z(0) \rangle \sim t^{-\alpha}$  with exponent  $\alpha$  close to 1/2 as expected for  $d = 1$ . At low temperatures, the diffusive contribution was practically undetectable.<sup>12</sup> Meanwhile, nuclear magnetic resonance (NMR)<sup>24</sup> and muon spin relaxation<sup>25</sup> experiments even found evidence for *low-temperature diffusive behavior* in  $S = 1/2$  Heisenberg chains, but have so far remained unexplained.

## II. FIELD THEORY AND EXPERIMENT

In the NMR experiment on the spin chain compound  $\text{Sr}_2\text{CuO}_3$ , spin diffusion is observed as a characteristic

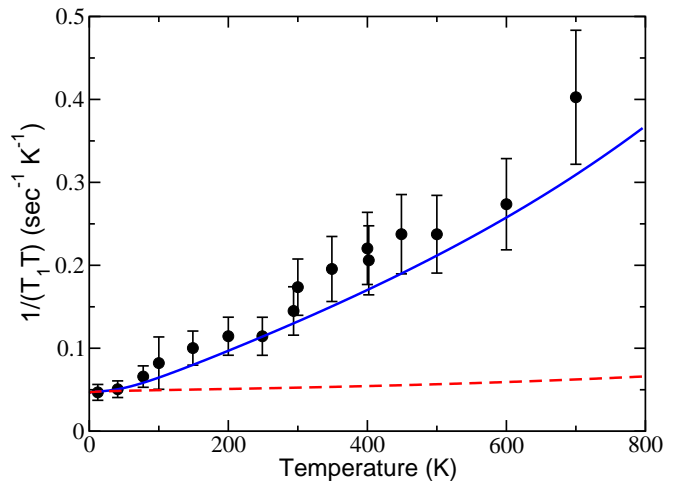


FIG. 2: Experimental data for the spin-lattice relaxation rate of the spin chain compound  $\text{Sr}_2\text{CuO}_3$  at  $h = 9$  T taken from Ref. [24] (dots) compared to our theory (blue solid line). Without diffusion,  $\gamma = 0$ ,  $1/(T_1 T)$  would be almost constant (red dashed line). The curves shown are obtained for  $J = 2000$  K and  $A$  as given in appendix D.

magnetic field dependence of the spin lattice relaxation rate,  $1/T_1 \sim 1/\sqrt{h}$ .<sup>24</sup> Here, only excitations with momentum  $q \sim 0$ , relevant for the studied transport properties, contribute. Clearly,  $\text{Sr}_2\text{CuO}_3$  is not exactly an integrable system. However, the behavior is expected to be different depending on whether the diffusion constant is determined by intrinsic umklapp scattering within the integrable model or by integrability-breaking perturbations. The spin excitations propagating in a given channel only contribute to the diffusive response at frequencies which are small compared to the relaxation rate in that channel. If the Drude weight of the XXZ model is large in the regime  $h \ll T \ll J$ , then we expect a large fraction of the excitations in  $\text{Sr}_2\text{CuO}_3$  to propagate in a quasi-ballistic channel with a very small relaxation rate. The diffusive response should therefore be suppressed compared to the case where the integrable model has a dominant diffusive channel.

We now calculate  $1/T_1$  by a standard field theory approach based on the Luttinger model<sup>17</sup> assuming that there is no unknown nonlocal conservation law. For the pure Luttinger model,  $1/T_1 \sim T$  in the limit  $T \rightarrow 0$ .<sup>26</sup> A finite decay rate  $\gamma(T)$  is obtained at second order in the umklapp scattering amplitude as displayed in appendix B and appendix D. For the Heisenberg model ( $\Delta = 1$ ) at half-filling, we find  $\gamma \sim T/\ln^2(J/T)$ . This implies spin diffusion in the sense that  $\langle n_l(t) n_l(0) \rangle \sim T\sqrt{\gamma/t}$  at large times. At high temperatures such that  $\gamma \gg h$  but still  $T \ll J$ , we find  $1/T_1 \sim T\sqrt{\gamma/h}$ . A comparison of the essentially parameter-free calculated temperature dependence with experiment is shown in Fig. 2. The good agreement indicates that a large diffusive response

is present in the integrable model near half-filling. Furthermore, this result shows that umklapp scattering is a “dangerously irrelevant” perturbation of the Luttinger model,<sup>26</sup> completely changing the behavior of  $1/T_1$  in the regime  $\hbar \ll T$  from a constant to a square-root divergence  $1/\sqrt{\hbar}$ , as seen in experiment.

Our field theory calculation assumed  $D(T > 0) = 0$ . In this case, the optical conductivity is a Lorentzian with width set by  $\gamma$ . If conservation laws protecting the Drude weight are present, they can be naturally incorporated using the memory matrix formalism.<sup>2</sup> But in this case spectral weight would be shifted from the Lorentzian into a ballistic part that does not contribute to the temperature dependence of  $1/(T_1 T)$  (see equation (F18)). That the experimental points in Fig. 2 are actually mostly *above* the theoretical prediction suggests that  $D$  is rather small near half-filling. Additional sources for diffusion, as for example phonons, might explain why our theory does not fully account for the temperature dependence of  $1/(T_1 T)$ .

### III. NUMERICAL RESULTS

In order to clarify the contradiction with previous studies that supported a large Drude weight at half-filling,<sup>7,8</sup> we used a DMRG algorithm<sup>12,23</sup> to calculate the current-current correlation directly in the thermodynamic limit. Fig. 3(a) shows numerical results for  $\langle j_l(t)j_0(0) \rangle$  at  $T = \infty$ . By summing over sites  $l$ , we obtain  $C(t) \equiv \langle \mathcal{J}(t)\mathcal{J} \rangle / L$  which asymptotically yields  $D$  according to equation (1). Remarkably, the results in Fig. 3(b) show that  $C(t)$  is nonmonotonic and does not converge to an asymptotic value for times up to  $Jt = 11$ . This is true within the critical as well as the gapped regime. We conclude that a large time scale persists at  $T = \infty$ . As stated in [8], exact diagonalization data should not be used to speculate about the Drude weight

in the thermodynamic limit at low temperatures, where a large length scale (mean free path) surely exists. Our results show that finite size data for the integrable model at half-filling are not reliable even at infinite temperature.

Furthermore, we have verified that the QMC results<sup>5</sup> cannot resolve the small decay rate  $\gamma(T) \ll T$  and cannot be used to conclude that  $D$  is finite. To further support that  $\gamma(T)$  is nonzero for  $T \ll J$ , we show  $C(t)/2JT$  at  $T = 0.2J$  in Fig. 3(c). At intermediate times  $J^{-1} \ll t \ll 1/\gamma$ , we expect that  $C(t)/2JT$  decays linearly with a slope proportional to  $\gamma$  (see equation (F21)). A linear fit in this regime yields values which are consistent with our theory (see Fig. 3(d)). We also note that the values of  $C(t)/2JT$  for  $Jt \approx 6$  are already smaller than the Drude weight found in [10] by BA.

### IV. CONCLUSIONS

To summarize, we have shown that in integrable 1D systems diffusion can coexist with ballistic transport, in the sense illustrated in Fig. 1. This is the scenario for the XXZ model away from half-filling. For the half-filled case, however, we have argued that the large diffusive response measured experimentally in spin chains and seen in our numerical calculations suggests that, contrary to common belief, the low-temperature Drude weight is either zero or surprisingly small.

### Acknowledgments

The authors thank A. Alvarez and C. Gros for sending us their quantum Monte Carlo data and acknowledge valuable discussions with T. Imai, A. Klümper and A. Rosch. This research was supported by NSERC (J.S., R.G.P., I.A.), CIFAR (I.A.), and the NSF under Grant No. PHY05-51164 (R.G.P.).

### APPENDIX A: LOW ENERGY EFFECTIVE MODEL

Bosonization of the XXZ model, equation (2), in the gapless regime at half-filling leads to the effective Hamiltonian<sup>17,27,28</sup>

$$\begin{aligned} H &= H_0 + H_u + H_{bc}, \\ H_0 &= \frac{v}{2} \int dx [\Pi^2 + (\partial_x \phi)^2], \\ H_u &= \lambda \int dx \cos(\sqrt{8\pi K} \phi), \\ H_{bc} &= -2\pi v \lambda_+ \int dx (\partial_x \phi_R)^2 (\partial_x \phi_L)^2 - 2\pi v \lambda_- \int dx [(\partial_x \phi_R)^4 + (\partial_x \phi_L)^4]. \end{aligned} \quad (\text{A1})$$

Here,  $H_0$  is the standard Luttinger model and  $H_u$  and  $H_{bc}$  are the leading irrelevant perturbations due to umklapp scattering and band curvature, respectively. The bosonic field  $\phi = \phi_R + \phi_L$  and its conjugate momentum  $\Pi$  obey the canonical commutation relation  $[\phi(x), \Pi(x')] = i\delta(x - x')$ . The long-wavelength ( $q \sim 0$ ) fluctuation part of the

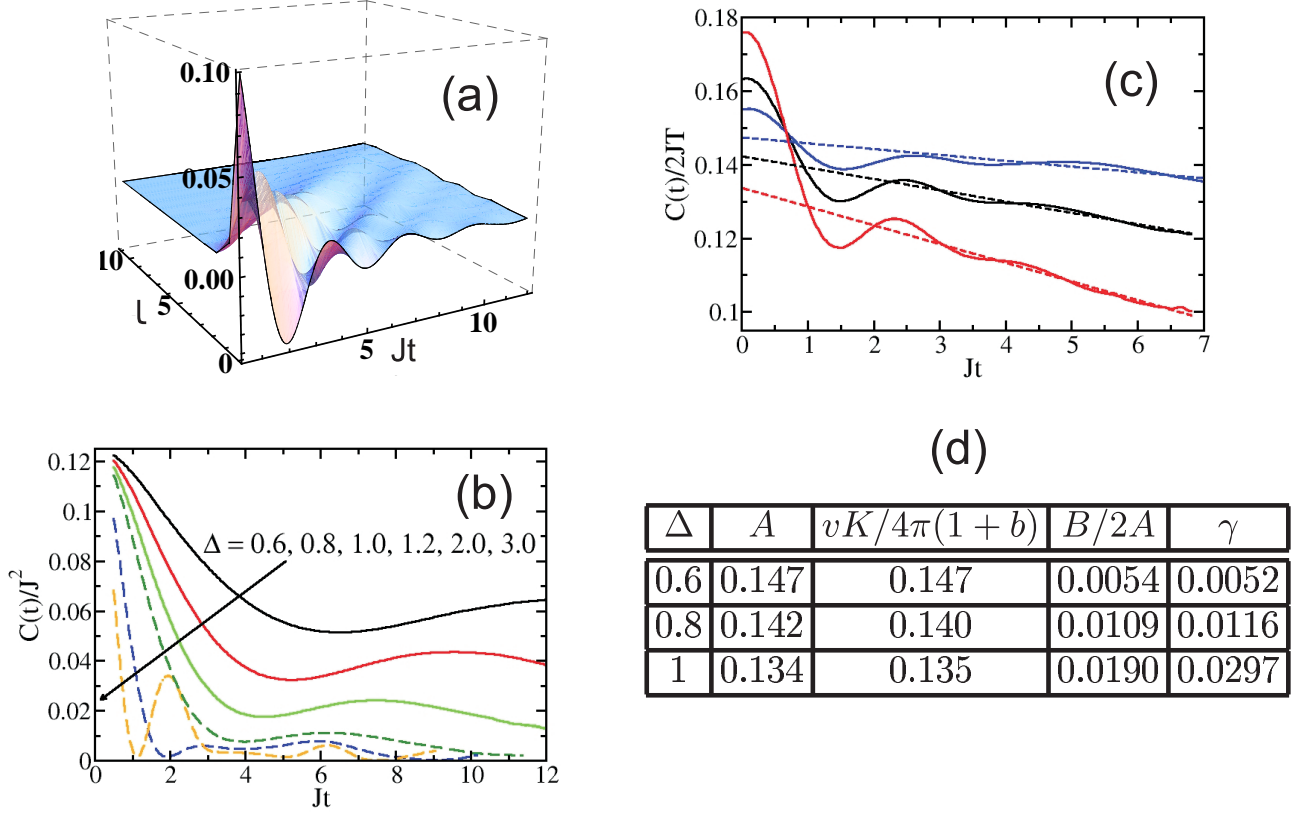


FIG. 3: (a)  $\langle j_l(t)j_0(0) \rangle$  for  $\Delta = 0.8$  and  $T = \infty$ . The wave fronts travel with a velocity  $v_\infty \approx 1.2J$ . (b)  $C(t) = \langle \mathcal{J}(t)\mathcal{J}(0) \rangle / L$  at infinite temperatures for various  $\Delta$  as indicated on the plot. The solid (dashed) lines correspond to  $\Delta$  in the critical (gapped) regime, respectively. (c)  $C(t)/2JT$  at  $T = 0.2J$  for  $\Delta = 0.6$  (blue solid line),  $\Delta = 0.8$  (black solid line), and  $\Delta = 1.0$  (red solid line). The dashed lines are linear fits  $C(t)/2JT = A - BJt$  for  $Jt \in [3.5, 7]$ . (d) The fitted values in comparison to theory. We expect  $A = vK/4\pi(1+b)$  and  $B/2A = \gamma$ . Note that a small Drude weight is not detectable in this linear regime (see appendix F).

fermion density is related to the bosonic field by  $n_j \sim \sqrt{K/2\pi} \partial_x \phi$ . The spin velocity and the Luttinger parameter  $K$  are known exactly from Bethe ansatz:

$$v = \frac{\pi \sqrt{1 - \Delta^2}}{2 \arccos \Delta} \quad ; \quad K = \frac{\pi}{\pi - \arccos \Delta} . \quad (\text{A2})$$

In this notation,  $K = 2$  at the free fermion point ( $\Delta = 0$ ) and  $K = 1$  at the isotropic point ( $\Delta = 1$ ). The amplitudes  $\lambda$ ,  $\lambda_+$ , and  $\lambda_-$  are also known exactly<sup>28</sup>:

$$\begin{aligned} \lambda &= \frac{K\Gamma(K) \sin(\pi/K)}{\pi\Gamma(2-K)} \left[ \frac{\Gamma\left(1 + \frac{1}{2K-2}\right)}{2\sqrt{\pi}\Gamma\left(1 + \frac{K}{2K-2}\right)} \right]^{2K-2}, \\ \lambda_+ &= \frac{1}{2\pi} \tan \frac{\pi K}{2K-2}, \\ \lambda_- &= \frac{1}{12\pi K} \frac{\Gamma\left(\frac{3K}{2K-2}\right) \Gamma^3\left(\frac{1}{2K-2}\right)}{\Gamma\left(\frac{3}{2K-2}\right) \Gamma^3\left(\frac{K}{2K-2}\right)}. \end{aligned} \quad (\text{A3})$$

## APPENDIX B: RETARDED SPIN-SPIN CORRELATION FUNCTION

In terms of spin-1/2 operators, the XXZ model in a longitudinal field  $h$  reads

$$H = \sum_{l=1}^N [J(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z) - \mu_B h S_l^z], \quad (\text{B1})$$

where  $\mu_B$  is the Bohr magneton. The spin operators are related to the spinless fermions by the usual Jordan-Wigner transformation. In particular, the  $z$  component is mapped to the local density of fermions,  $S_j^z \sim n_j - 1/2$ . We are interested in the retarded spin-spin correlation function  $\chi_{\text{ret}}(q, \omega)$ , which can be obtained from the Matsubara correlation function

$$\chi(q, i\omega_n) = -\frac{1}{N} \sum_{l, l'} e^{-iq(l-l')} \int_0^{1/T} d\tau e^{i\omega_n \tau} \langle S_l^z(\tau) S_{l'}^z(0) \rangle \quad (\text{B2})$$

by the analytic continuation  $i\omega_n \rightarrow \omega + i0^+$ .

In the low-energy limit, we follow ref. [29] and relate the long-wavelength part of the retarded spin-spin correlation function to the boson propagator

$$\frac{\chi_{\text{ret}}(q, \omega)}{Kq^2/2\pi} = \langle \phi \phi \rangle^{\text{ret}}(q, \omega) = \frac{v}{\omega^2 - v^2 q^2 - \Pi^{\text{ret}}(q, \omega)}. \quad (\text{B3})$$

We calculate the self-energy  $\Pi^{\text{ret}}(q, \omega) = \Pi_{\text{u}}^{\text{ret}}(q, \omega) + \Pi_{\text{bc}}^{\text{ret}}(q, \omega)$  by perturbation theory to second order in  $H_{\text{u}}$  and first order in  $H_{\text{bc}}$ . In the following, we focus on the half-filling case ( $h = 0$ ).

The contribution from umklapp scattering reads

$$\Pi_{\text{u}}^{\text{ret}}(q, \omega) = 4\pi K v \lambda^2 [F^{\text{ret}}(q, \omega) - F^{\text{ret}}(0, 0)], \quad (\text{B4})$$

where<sup>30</sup>

$$F^{\text{ret}}(q, \omega) = -\frac{v}{T^2} \left( \frac{\pi T}{v} \right)^{4K} \sin(2\pi K) I\left(\frac{\omega + vq}{2T}\right) I\left(\frac{\omega - vq}{2T}\right),$$

with

$$I(z) = \int_0^\infty \frac{e^{izu} du}{\sinh^{2K}(\pi u)} = \frac{2^{2K-1}}{\pi} B\left(K - \frac{iz}{2\pi}, 1 - 2K\right), \quad (\text{B5})$$

where  $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$  is the beta function. For  $K > 1/2$ , we need a cutoff in the integral  $I(z)$  in equation (B5). However, the imaginary part of  $I(z)$  does not depend on the cutoff scheme used.<sup>30</sup> The expansion of equation (B5) for  $|\omega \pm vq| \ll T$  yields both a real and an imaginary part for  $\Pi_{\text{u}}^{\text{ret}}(q, \omega)$ . The calculation of  $\Pi_{\text{bc}}^{\text{ret}}(q, \omega)$  is also standard. By contrast with  $\Pi_{\text{u}}^{\text{ret}}(q, \omega)$ , the result for  $\Pi_{\text{bc}}^{\text{ret}}(q, \omega)$  is purely real, as band curvature terms do not contribute to the decay rate. The end result is

$$\Pi^{\text{ret}}(q, \omega) \approx -2i\gamma\omega - b\omega^2 + cv^2q^2, \quad (\text{B6})$$

with parameters

$$\begin{aligned} 2\gamma &= Y_1 T^{4K-3} \\ b &= \underbrace{(Y_2 - Y_3) T^{4K-4}}_{b_2} + \underbrace{Y_4 T^2}_{b_1} \\ c &= \underbrace{-(Y_2 + Y_3) T^{4K-4}}_{c_2} - \underbrace{Y_4 T^2}_{c_1} \end{aligned} \quad (\text{B7})$$

$$\begin{aligned}
Y_1 &= \Lambda \frac{B(K, 1-2K)}{\sqrt{\pi} 2^{2K+1}} \cot(\pi K), \\
Y_2 &= \Lambda \frac{B(K, 1-2K)}{\pi^{5/2} 2^{2K+4}} (\pi^2 - 2\Psi'(K)), \\
Y_3 &= \Lambda \frac{1}{\pi 2^{4K+4}} \cot^2(\pi K) \Gamma(1/2 - K) \Gamma(K), \\
Y_4 &= \frac{\pi^2}{6v^2} (\lambda_+ + 6\lambda_-), \\
\Lambda &= 4\pi K \lambda^2 \sin(2\pi K) \left( \frac{2\pi}{v} \right)^{4K-2} \Gamma(1/2 - K) \Gamma(K).
\end{aligned} \tag{B8}$$

Here  $b_1$  and  $c_1$  ( $b_2$  and  $c_2$ ) are the parts stemming from the band curvature (umklapp) terms, respectively.

At the isotropic point,  $\Delta = 1$ , umklapp scattering becomes marginal and logarithmic corrections have to be taken into account. In this case we find

$$\begin{aligned}
2\gamma &= \pi g^2 T, \\
b &= \frac{g^2}{4} - \frac{g^3}{32} \left( 3 - \frac{8\pi^2}{3} \right) + \frac{\sqrt{3}}{\pi} T^2, \\
c &= \frac{g^2}{4} - \frac{3g^3}{32} - \frac{\sqrt{3}}{\pi} T^2.
\end{aligned} \tag{B9}$$

Following Lukyanov,<sup>28</sup> the running coupling constant  $g(T)$  is determined by the equation

$$\frac{1}{g} + \frac{\ln g}{2} = \ln \left[ \sqrt{\frac{\pi}{2}} \frac{e^{1/4+\tilde{\gamma}}}{T} \right], \tag{B10}$$

where  $\tilde{\gamma}$  is the Euler constant. We remark that a similar calculation was attempted in ref. [3], but there the imaginary part of the self-energy was neglected.

### APPENDIX C: SPIN DIFFUSION

In this section we consider the long-time behavior of the spin-spin correlation function  $\langle S_{l+x}^z(t) S_l^z(0) \rangle$  at half-filling. At zero temperature, it is known<sup>31</sup> that the slowest decaying term in the autocorrelation function for  $0 < \Delta < 1$  is of the form

$$\langle S_l^z(t) S_l^z(0) \rangle \sim \frac{e^{-iWt}}{t^\eta}, \quad (T = 0) \tag{C1}$$

with  $W = v$  and  $\eta = (K + 1)/2$ . This oscillating term is attributed to  $q = \pi/2$  high-energy particle-hole excitations with a hole near the bottom of the band and a particle at the Fermi surface, or a particle at the top of the band and a hole at the Fermi surface. At  $T = 0$ , the low-energy contributions to the spin-spin correlation function decay faster than the high-energy contributions. In contrast, numerical studies show that at high temperatures the oscillating terms are still present, but the slowest decaying term has pure power-law decay with no oscillations.<sup>11,12</sup> This slow decaying term has been interpreted as due to spin diffusion at high temperatures. Here we will show that a diffusive term is already present at low temperatures. In the following we use the boson propagator in equation (B3) to calculate the  $q \sim 0$  low-energy contribution to the autocorrelation function in the regime  $T \ll J$ .

We can write the low-energy, long-wavelength contribution to  $\langle S_{l+x}^z(t) S_l^z(0) \rangle$  as

$$G(x, t) \equiv -2 \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{+\infty} \frac{dq}{2\pi} e^{i(qx - \omega t)} \frac{\text{Im} \chi_{\text{ret}}(q, \omega)}{1 - e^{-\omega/T}}, \tag{C2}$$

with  $\chi_{\text{ret}}(q, \omega)$  given by equation (B3). Doing the integral over  $q$  first, we find

$$G(x, t) = \frac{K}{2\pi v^2} (1+b)^{-1/2} (1+c)^{-3/2} \int_{-\infty}^{+\infty} \frac{d\tilde{\omega}}{4\pi} \exp[-i\tilde{\omega}\tilde{t} - i(\tilde{\omega}^2 + 2i\tilde{\gamma}\tilde{\omega})^{1/2} |\tilde{x}|/v] \frac{(\tilde{\omega}^2 + 2i\tilde{\gamma}\tilde{\omega})^{1/2}}{1 - e^{-\tilde{\omega}/\tilde{T}}} - (\tilde{\gamma} \rightarrow -\tilde{\gamma}), \tag{C3}$$

where  $\tilde{t} = t(1+b)^{-1/2}$ ,  $\tilde{x} = x(1+c)^{-1/2}$ ,  $\tilde{\gamma} = \gamma(1+b)^{-1/2}$  and  $\tilde{T} = T(1+b)^{1/2}$ . The integral in equation (C3) has both pole and branch cut contributions. We assume  $\gamma \ll T$  at low temperatures. In the limit  $t \gg 1/\gamma$ , we find

$$G(x, t) = (1+b)^{-1/2}(1+c)^{-3/2}[G_0(x, t) + G_{\text{int}}(x, t)], \quad (\text{C4})$$

where

$$G_0(x, t) = \frac{K}{8\pi^2 v^2} \left\{ \frac{\pi \tilde{T}}{\sinh[\pi \tilde{T}(\tilde{t} - \tilde{x}/v)]} \right\}^2 + \frac{K}{8\pi^2 v^2} \left\{ \frac{\pi \tilde{T}}{\sinh[\pi \tilde{T}(\tilde{t} + \tilde{x}/v)]} \right\}^2 \quad (\text{C5})$$

is the Luttinger liquid result in terms of the rescaled variables and

$$G_{\text{int}}(x, t) = \frac{K \tilde{T}}{v^2} \sqrt{\frac{\gamma}{2\pi t}} e^{-\gamma \tilde{x}^2 / 2v^2 t} \quad (\text{C6})$$

is the diffusive term. Therefore, for all  $0 < \Delta \leq 1$ , at finite temperatures and sufficiently long times the autocorrelation function becomes dominated by a *low-energy* term

$$\langle S_l^z(t) S_l^z(0) \rangle \sim T \sqrt{\frac{\gamma(T)}{t}}, \quad (T \neq 0, t \gg 1/\gamma) \quad (\text{C7})$$

with the universal power-law decay  $t^{-1/2}$  expected for diffusion in one dimension.

#### APPENDIX D: SPIN-LATTICE RELAXATION RATE

The linear response formula for the spin-lattice relaxation rate is

$$\frac{1}{T_1} = \frac{1}{2} \int \frac{dq}{2\pi} |A(q)|^2 S^{+-}(q, \omega_N)|_h, \quad (\text{D1})$$

where  $A(q)$  is the hyperfine coupling form factor,  $\omega_N$  is the *nuclear* magnetic resonance frequency and

$$S^{+-}(q, \omega)|_h = \frac{1}{N} \sum_{l, l'} \int_{-\infty}^{+\infty} dt e^{i\omega_N t} \langle S_l^+(t) S_{l'}^-(0) \rangle|_h \quad (\text{D2})$$

is the transverse spin dynamical structure factor. Here  $S_l^\pm = S_l^x \pm iS_l^y$  are the raising and lowering spin operators. The expression in equation (D2) is to be calculated using Hamiltonian (B1) in the presence of a magnetic field  $h$ . We focus on the experimentally relevant Heisenberg point  $\Delta = 1$ . We would like to express  $1/T_1$  in terms of the longitudinal structure factor

$$S^{zz}(q, \omega) = \frac{1}{N} \sum_{l, l'} \int_{-\infty}^{+\infty} dt e^{i\omega_N t} \langle S_l^z(t) S_{l'}^z(0) \rangle \quad (\text{D3})$$

at zero field. The latter is more easily calculated in the field theory since  $S_l^z$  is related to the local density of fermions  $n_l$ , whereas  $S_l^\pm$  have nonlocal representations in terms of Jordan-Wigner fermions. Although the exchange term in the Heisenberg model is isotropic, the magnetic field term in equation (B1) breaks rotational symmetry. As a result,  $S^{+-}(q, \omega)|_h$  cannot be directly replaced by  $2S^{zz}(q, \omega)|_h$  at finite field. However, we note that the longitudinal field has a trivial effect on  $S_l^\pm(t)$

$$S_l^\pm(t) = e^{iHt} S_l^\pm e^{-iHt} = e^{-i\omega_e t} e^{i\bar{H}t} S_l^\pm e^{-i\bar{H}t}, \quad (\text{D4})$$

where  $\bar{H} = H(h = 0)$  and  $\omega_e = \mu_B h$  is the *electron* magnetic resonance frequency. If we assume in addition that  $T \gg \omega_e$ , the magnetic field dependence in the thermal average can be neglected and we have

$$S^{+-}(q, \omega)|_h \approx \frac{2}{N} \sum_{l, l'} \int_{-\infty}^{+\infty} dt e^{i(\omega_N - \omega_e)t} \langle S_l^z(t) S_{l'}^z(0) \rangle|_0, \quad (\text{D5})$$

where the correlation function is calculated at  $\hbar = 0$ . This leads to the expression for the spin-lattice relaxation rate

$$\frac{1}{T_1} \approx \int \frac{dq}{2\pi} |A(q)|^2 S^{zz}(q, \omega_N - \omega_e)|_0. \quad (\text{D6})$$

Using  $\omega_e \gg \omega_N$  and

$$S^{zz}(q, -\omega_e) = \frac{2\text{Im } \chi_{\text{ret}}(q, \omega_e)}{1 - e^{\omega_e/T}}, \quad (\text{D7})$$

we find in the regime  $\omega_e \ll T$

$$\frac{1}{T_1} \approx -\frac{2T}{\omega_e} \int \frac{dq}{2\pi} |A(q)|^2 \text{Im } \chi_{\text{ret}}(q, \omega_e). \quad (\text{D8})$$

For the in-chain oxygen site in  $\text{Sr}_2\text{CuO}_3$ , we have  $A(q) = A \cos(q/2)$  with

$$|A|^2 = \frac{k_B}{2\hbar} \frac{(2C^b)^2 + (2C^c)^2}{\pi^3 k_B^2 J^2} (g\gamma_N \hbar)^2, \quad (\text{D9})$$

where  $k_B$  is the Boltzmann constant,  $C^{b,c}$  are the dimensionless components of the hyperfine coupling tensor,<sup>24</sup>  $g\gamma_N \hbar = 4.74 \times 10^{-9}$  eV and  $J$  is the exchange coupling measured in Kelvin.

At low temperatures  $T \ll J$ , the integral in equation (D8) is dominated by the  $q \sim 0$  mode of  $\chi_{\text{ret}}(q, \omega)$ . Performing the momentum integral using the retarded correlation function in equation (B3) with the appropriate parameters (B9) for the isotropic case yields

$$\frac{1}{T_1 T} = \frac{k_B}{\hbar} \frac{(2C^b)^2 + (2C^c)^2}{\pi^3 k_B^2 J^2} (g\gamma_N \hbar)^2 X_1 \sqrt{\frac{X_2}{2} + \sqrt{\left(\frac{X_2}{2}\right)^2 + \left(\frac{\gamma}{\omega_e}\right)^2}}, \quad (\text{D10})$$

where

$$\begin{aligned} X_1 &= 1 + \frac{g}{2} - \frac{g^2}{8} + \frac{5g^3}{64} + \frac{3\sqrt{3}}{2\pi} T^2, \\ X_2 &= 1 + \frac{g^2}{4} - \frac{g^3}{32} \left(3 - \frac{8\pi^2}{3}\right) + \frac{\sqrt{3}}{\pi} T^2. \end{aligned} \quad (\text{D11})$$

In the limit  $\gamma(T) \gg \omega_e$ , we obtain the diffusive behavior

$$\frac{1}{T_1 T} \sim \sqrt{\frac{\gamma(T)}{\omega_e}} \sim \sqrt{\frac{T/\ln^2(J/T)}{\omega_e}}. \quad (\text{D12})$$

We note that the temperature dependence of the effective diffusion constant  $D_s \equiv v^2/2\gamma$  is different from the one proposed in ref. [24].

From a fit of the experimental susceptibility data obtained in refs. [24,32] using the full parameter-free field theory<sup>28,33</sup> we obtain  $J = 2000 \pm 200$  K. The components of the hyperfine coupling tensor, on the other hand, are given by  $2C^b = 95 \pm 10$  and  $2C^c = 44 \pm 10$ .<sup>24</sup> To obtain the curve shown in Fig. 3 we used  $J = 2000$  K and  $2C^b = 105$ , and  $2C^c = 54$ . The dashed line in Fig. 3 was obtained by setting  $\gamma = 0$  in equation (D10) while keeping the temperature dependence in the parameters  $X_1$  and  $X_2$ . This would correspond to purely ballistic transport with a temperature-dependent Drude weight as suggested by the Bethe ansatz calculation of ref. [10]. The figure shows that a large low-temperature Drude weight cannot be consistent with the temperature dependence of the spin-lattice relaxation rate.

## APPENDIX E: FINITE MAGNETIC FIELDS AND THE MAZUR BOUND

The current density operator is defined from the continuity equation for the fermion density

$$\partial_t n_l = -i[n_l, H] = -(j_l - j_{l-1}), \quad (\text{E1})$$



which for the XXZ model yields

$$j_l = -\frac{iJ}{2}(c_l^\dagger c_{l+1} - c_{l+1}^\dagger c_l). \quad (\text{E2})$$

Away from half-filling, the integrated current operator  $\mathcal{J} = \sum_l j_l$  has a finite overlap with the local conserved quantities of the XXZ model. The simplest nontrivial conserved quantity is

$$\mathcal{J}_E = i\frac{J^2}{2} \sum_l \left[ \frac{1}{2}(c_{l-1}^\dagger c_{l+1} - c_{l+1}^\dagger c_{l-1}) - \Delta(c_{l-1}^\dagger c_l - c_l^\dagger c_{l-1}) \left( n_{l+1} - \frac{1}{2} \right) + \left( n_{l-1} - \frac{1}{2} \right) (c_l^\dagger c_{l+1} - c_{l+1}^\dagger c_l) \right]. \quad (\text{E3})$$

Here  $\mathcal{J}_E$  is the energy current operator as obtained from the continuity equation for the Hamiltonian density.<sup>6</sup> It can be verified that  $\mathcal{J}_E$  is conserved in the sense that  $[\mathcal{J}_E, H] = 0$ . According to Mazur's inequality, equation (1), the overlap of  $\mathcal{J}$  with  $\mathcal{J}_E$  provides a lower bound for the Drude weight:

$$D \geq D_{\text{Mazur}} \equiv \frac{1}{2TL} \frac{\langle \mathcal{J} \mathcal{J}_E \rangle^2}{\langle \mathcal{J}_E^2 \rangle}. \quad (\text{E4})$$

The Mazur bound in the limit  $T \rightarrow \infty$  was calculated in ref. [6]

$$D_{\text{Mazur}} = \frac{J}{T} \frac{4\Delta^2 m^2 (1/4 - m^2)}{1 + 8\Delta^2 (1/4 + m^2)} \quad (T \gg J), \quad (\text{E5})$$

where  $m = \langle S_l^z \rangle = \langle n_l \rangle - 1/2$  is the magnetization in the spin model.

In the gapless phase, the Mazur bound can also be calculated in the low-temperature regime using the field theory representations of  $\mathcal{J}$  and  $\mathcal{J}_E$ . In the continuum limit, the continuity equation becomes

$$\partial_t n(x) + \partial_x j(x) = 0.$$

Using the bosonized form  $n(x) = \sqrt{K/2\pi} \partial_x \phi$ , we obtain for effective model (1)

$$\mathcal{J} = -\sqrt{\frac{K}{2\pi}} \int dx \partial_t \phi = -v \sqrt{\frac{K}{2\pi}} \int dx \left[ \Pi - \frac{\pi}{2} (\lambda_+ + 2\lambda_-) \Pi^3 - \frac{\pi}{2} (-\lambda_+ + 6\lambda_-) \Pi (\partial_x \phi)^2 \right]. \quad (\text{E6})$$

In the following we neglect the correction to the current operator due to band curvature terms and calculate the Mazur bound  $D_{\text{Mazur}}$  for the Luttinger model  $H_0$ :

$$\mathcal{J} \approx -v \sqrt{\frac{K}{2\pi}} \int dx \Pi. \quad (\text{E7})$$

The energy current operator for the Luttinger model is

$$\mathcal{J}_E \approx -v^2 \int dx \Pi \partial_x \phi. \quad (\text{E8})$$

At half-filling, the overlap vanishes because  $\mathcal{J}$  and  $\mathcal{J}_E$  have opposite signatures under the particle-hole transformation  $\phi \rightarrow -\phi, \Pi \rightarrow -\Pi$ . Away from half-filling, a small magnetic field term in equation (B1) can be absorbed by shifting the bosonic field (here we set  $\mu_B = 1$ )

$$\phi \rightarrow \phi + \frac{h}{v} \sqrt{\frac{K}{2\pi}} x. \quad (\text{E9})$$

In this case, the conserved quantity becomes<sup>2</sup>

$$\tilde{\mathcal{J}}_E = -v^2 \int dx \Pi \partial_x \phi - hv \sqrt{\frac{K}{2\pi}} \int dx \Pi = \mathcal{J}_E + h\mathcal{J}. \quad (\text{E10})$$

We calculate the equal time correlations within the Luttinger model and find

$$D_{\text{Mazur}} = \frac{1}{2TL} \frac{\langle \mathcal{J} \tilde{\mathcal{J}}_E \rangle^2}{\langle \tilde{\mathcal{J}}_E^2 \rangle} = \frac{vK/4\pi}{1 + \frac{2\pi^2}{3K} \left( \frac{T}{h} \right)^2} \quad (T, h \ll J). \quad (\text{E11})$$

We note that in the limit  $T/h \rightarrow 0$  the Mazur bound obtained from the overlap with  $\tilde{\mathcal{J}}_E$  saturates the exact zero temperature Drude weight  $D(T=0) = vK/4\pi$ .<sup>18</sup>

One can also use the Bethe ansatz to calculate the Mazur bound in equation (E4) exactly. We computed the equal time correlations using a numerical solution of the nonlinear equations obtained within the Bethe ansatz formalism of refs. [34,35]. In Fig. 4, the numerical Bethe ansatz solution for small values of magnetization  $m$  is compared to the field theory formula (E11). Remarkably, the free boson result in equation (E11) fits well the behavior of the exact Mazur bound out to temperatures of order  $J$ .

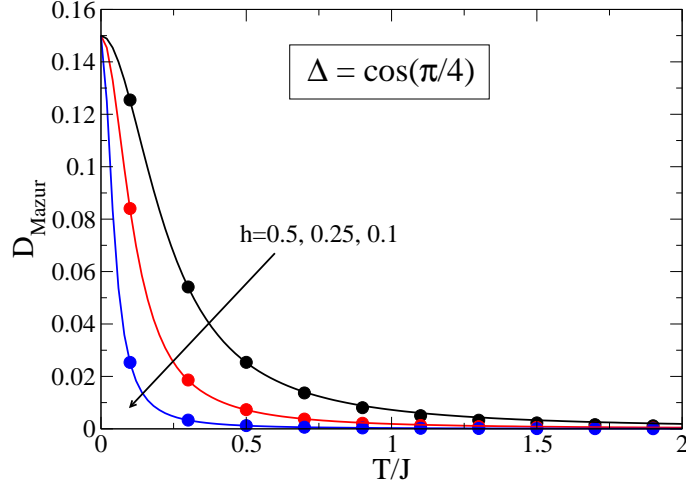


FIG. 4: Mazur bound  $D_{\text{Mazur}}$  as defined in (E4) calculated exactly using the Bethe ansatz (dots) compared to the field theoretical formula (E11) (lines).

## APPENDIX F: DECAY OF THE CURRENT-CURRENT CORRELATION FUNCTION

The time-dependent current-current correlation function can be written as

$$C(t) \equiv \frac{1}{L} \langle \mathcal{J}(t) \mathcal{J} \rangle = -2 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{1 - e^{-\omega/T}} \text{Im} \langle \mathcal{J}; \mathcal{J} \rangle_{\text{ret}}(\omega), \quad (\text{F1})$$

where  $\langle \mathcal{J}; \mathcal{J} \rangle_{\text{ret}}(\omega)$  is the retarded current-current correlation function. The latter appears in the Kubo formula for the optical conductivity

$$\sigma(\omega) = \frac{i}{\omega} \left[ \frac{\langle \mathcal{J}^2 \rangle}{LT} + \langle \mathcal{J}; \mathcal{J} \rangle_{\text{ret}}(\omega) \right], \quad (\text{F2})$$

where we used that the expectation value of the kinetic energy operator is given by  $-\langle \mathcal{J}^2 \rangle/T$  if the system has vanishing superfluid density. In the limit of small  $q$ , the Kubo formulated can be rewritten as<sup>3</sup>

$$\sigma(\omega) = \frac{K}{2\pi} i\omega \langle \phi \phi \rangle^{\text{ret}}(\omega). \quad (\text{F3})$$

If we apply the result from the self-energy approach in equation (B3), we have

$$\sigma(\omega) = \frac{vK}{2\pi} \frac{i\omega}{\omega^2 - \Pi(\omega)}. \quad (\text{F4})$$

In this case the real part of the conductivity is

$$\text{Re} \sigma(\omega) \equiv \sigma'(\omega) = \frac{vK}{2\pi} \frac{2\gamma}{[(1+b)\omega]^2 + (2\gamma)^2}. \quad (\text{F5})$$

The self-energy approach predicts zero Drude weight whenever  $\gamma(T)$  is nonzero. This result is inconsistent with Mazur's inequality if there exist conservation laws which protect the Drude weight. It is possible to accommodate the existence of nontrivial conservation laws by resorting to the memory matrix formalism of ref. [2]. This approach starts from the Kubo formula for a conductivity matrix  $\hat{\sigma}$  which includes not only the current operator  $\mathcal{J} \equiv \mathcal{J}_1$ , but also "slow modes"  $\mathcal{J}_n$  ( $n \geq 2$ ) which have a finite overlap with  $\mathcal{J}$ :

$$\sigma_{nm}(\omega) = \frac{i}{\omega} \left[ \frac{\langle \mathcal{J}_n \mathcal{J}_m \rangle}{LT} + \langle \mathcal{J}_n; \mathcal{J}_m \rangle_{\text{ret}}(\omega) \right]. \quad (\text{F6})$$

The conductivity in equation (F2) is the  $\sigma_{11}$  component of the conductivity matrix. The idea is that if  $\langle \mathcal{J}_n(t) \mathcal{J}_n(0) \rangle$  is a slowly decaying function of time, the projection of  $\mathcal{J}$  into  $\mathcal{J}_n$  governs the long-time behavior of the current-current correlation function and consequently dominates the low-frequency transport. The overlap between  $\mathcal{J}$  and

the slow modes is captured by the off-diagonal elements of the conductivity matrix. In practice, only a small number of conserved quantities is included in the set of slow modes, but the approach can be systematically improved since adding more conserved quantities increases the lower bound for the conductivity.<sup>36</sup>

It is convenient to invert the Kubo formula for the conductivity matrix using the projection operator method.<sup>36</sup> We introduce the scalar product between two operators  $A$  and  $B$  in the Liouville space

$$(A|B) = \frac{T}{L} \int_0^{1/T} d\tau \langle A^\dagger e^{H\tau} B e^{-H\tau} \rangle. \quad (\text{F7})$$

The susceptibility matrix  $\hat{\chi}$  is defined as

$$\chi_{nm} = T^{-1}(\mathcal{J}_n|\mathcal{J}_m). \quad (\text{F8})$$

We denote by

$$\mathcal{P} = 1 - T^{-1} \sum_{nm} \chi_{nm}^{-1} (\mathcal{J}_n)(\mathcal{J}_m| \quad (\text{F9})$$

the projector *out* of the subspace of slow modes. Using identities for the projection operator, equation (F6) can be brought into the form<sup>2</sup>

$$\sigma_{nm}(\omega) = i\{[\omega - \hat{M}\hat{\chi}^{-1}]^{-1}\hat{\chi}\}_{nm}, \quad (\text{F10})$$

where  $\hat{M}$  is the memory matrix given by

$$M_{nm} = T^{-1}(\mathcal{J}_n|\mathcal{L}\mathcal{P} \frac{1}{\omega - \mathcal{P}\mathcal{L}\mathcal{P}} \mathcal{P}\mathcal{L}|\mathcal{J}_m). \quad (\text{F11})$$

Here,  $\mathcal{L}$  is the Liouville superoperator defined by  $\mathcal{L}\mathcal{J}_n = [H, \mathcal{J}_n]$ . For simplicity, we assumed that all the slow modes have the same signature under time-reversal symmetry. It can be shown that if there is an exact conservation law (local or nonlocal) involving one of the slow modes, the memory matrix has a vanishing eigenvalue, which then implies a finite Drude weight. In the following we apply the memory matrix formalism to calculate the conductivity for the low-energy effective model (A1) at half-filling, allowing for the existence of a single conserved quantity  $Q$ ,  $[Q, H] = 0$ . The conductivity matrix is then two-dimensional. We choose  $\mathcal{J}_1 = \mathcal{J}$  and  $\mathcal{J}_2 = Q_\perp \equiv Q - \mathcal{J}(\mathcal{J}|Q)(\mathcal{J}|\mathcal{J})^{-1}$  so that  $\hat{\chi}$  is diagonal. At low temperatures  $T \ll J$ , we can use the current operator in equation (E6); to first order in  $\lambda_\pm$ , we obtain

$$\chi_{11} \approx \frac{\langle \mathcal{J}^2 \rangle}{LT} \approx \frac{vK}{2\pi}(1 - b_1), \quad (\text{F12})$$

where  $b_1$  is defined in equation (B7). Likewise,  $\chi_{22} = (\langle Q^2 \rangle - \langle Q\mathcal{J} \rangle^2 / \langle \mathcal{J}^2 \rangle) / (LT)$  can be calculated within the low energy effective model once a conserved quantity  $Q$  has been identified. The remaining approximation is in the calculation of the memory matrix to second order in umklapp. This is analogous to the calculation of the self-energy  $\Pi_u^{\text{ret}}$  in equation (B4). Using the conservation law, we can write

$$\hat{M} \approx M_{11}(\omega) \begin{pmatrix} 1 & -r \\ -r & r^2 \end{pmatrix}, \quad (\text{F13})$$

where  $r = \langle Q\mathcal{J} \rangle / \langle \mathcal{J}^2 \rangle$  and

$$M_{11}(\omega) \approx \frac{vK}{2\pi} \frac{\Pi_u(\omega)}{\omega} \approx \frac{vK}{2\pi} (-b_2\omega - 2i\gamma), \quad (\text{F14})$$

with  $b_2$  as given in equation (B7). Thus, from equation (F10), we find

$$\sigma(\omega) = \chi_{11} \left[ \frac{y}{1+y} \frac{i}{\omega} + \frac{1}{1+y} \frac{i}{\omega - (1+y)\chi_{11}^{-1}M_{11}(\omega)} \right], \quad (\text{F15})$$

where

$$y = \frac{r^2\chi_{11}}{\chi_{22}} = \frac{\langle \mathcal{J}Q \rangle^2}{\langle \mathcal{J}^2 \rangle \langle Q^2 \rangle - \langle \mathcal{J}Q \rangle^2}. \quad (\text{F16})$$

Equating equations (F4) and (F15), we find that the memory matrix approach is equivalent to adopting the self-energy

$$\Pi(\omega) \approx \frac{\omega \chi_{11}^{-1} M_{11}(\omega) - b_1 \omega^2}{1 - y \chi_{11}^{-1} M_{11}(\omega)/\omega} = \frac{-b\omega^2 - 2i\gamma\omega}{1 - y \chi_{11}^{-1} M_{11}(\omega)/\omega}. \quad (\text{F17})$$

As expected, the memory matrix result reduces to the self-energy result for  $y \rightarrow 0$ . The difference between the self-energy and the memory matrix result is of higher order in the umklapp interaction. Therefore, the conservation law is not manifested in the lowest-order calculation of the self-energy. Although equation (F17) is not correct beyond  $O(\lambda^2, \lambda_\pm)$ , it suggests that the memory matrix approach corresponds to a partial resummation of an infinite family of Feynman diagrams which changes the behavior of  $\Pi(\omega)$  in the limit  $\omega \rightarrow 0$  from  $\Pi \rightarrow -2i\gamma\omega$  to  $\Pi \rightarrow -y^{-1}\omega^2$ .

It follows from equation (F2) that

$$\text{Im}\langle \mathcal{J}; \mathcal{J} \rangle_{\text{ret}}(\omega) = -\omega \text{Re} \sigma(\omega) = -\omega \frac{vK}{2\pi} \left[ \frac{\pi y(1-b_1)}{1+y} \delta(\omega) + \frac{2\gamma}{(1+b_1+b'_2)^2\omega^2 + (2\gamma')^2} \right]. \quad (\text{F18})$$

where  $b'_2 = (1+y)b_2$  and  $\gamma' = (1+y)\gamma$ . The first term on the right hand side of equation (F18) can be associated with the ballistic channel and the second one with the diffusive channel. Substituting equation (F18) into equation (F1) and computing the integral, we find that for times  $t \gg (2\pi T)^{-1}$

$$C(t) \sim \frac{vKT}{2\pi(1+y)} \left( y(1-b_1) + \frac{e^{-2\gamma't}}{1+b_1+b'_2} \right). \quad (\text{F19})$$

Therefore, in the limit  $t \rightarrow \infty$  the current-current correlation function approaches the value

$$\lim_{t \rightarrow \infty} C(t) = \frac{vKT y(1-b_1)}{2\pi(1+y)} \approx \frac{\langle \mathcal{J}^2 \rangle y}{L(1+y)} = \frac{\langle \mathcal{J}Q \rangle^2}{L\langle Q^2 \rangle}, \quad (\text{F20})$$

consistent with the Mazur bound for the Drude weight.

For intermediate times  $(2\pi T)^{-1} \ll t \ll 1/\gamma'$ , we obtain the linear decay

$$C(t) \approx \frac{vKT}{2\pi(1+b)}(1-2\gamma t), \quad (\text{F21})$$

independent of  $y$  if  $b_1, b'_2 \ll 1$ . Therefore a small Drude weight cannot be detected in this intermediate time range. However, we can extract the decay rate  $\gamma$  by fitting the numerical results for  $C(t)$  at low temperatures (see table in fig. 3).

In addition to the data shown in Fig. 3, we also calculated  $C(t)$  at relatively large magnetic fields and various temperatures. As shown in Fig. 5 we find that in this case  $C(t)$  appears to converge to a finite value within fairly short times. Furthermore, we find (see Fig. 6) that at large  $\Delta$  and large magnetic fields the Mazur bound (E5) almost completely exhausts the Drude weight at high temperatures. This is consistent with the findings in ref. [6] which were based on exact diagonalization.

## APPENDIX G: COMPARISON WITH QUANTUM MONTE CARLO

It follows from equation (B3) that the dynamical conductivity  $\sigma(q, \omega_n)$  defined in ref. [5,37] is given by

$$\sigma(q, \omega_n) = -\frac{\omega_n}{q^2} \chi_{\text{ret}}(q, i\omega_n) = \frac{vK}{2\pi} \frac{\omega_n}{(1+b)\omega_n^2 + (1+c)v^2q^2 + 2\gamma\omega_n}. \quad (\text{G1})$$

Here,  $\omega_n$  are Matsubara frequencies. The function  $\sigma(q, \omega_n)$  can be calculated numerically by quantum Monte Carlo (QMC). By fitting the numerical results, one tries to extract a possible nonzero relaxation rate  $\gamma$ . If  $\gamma = 0$ , one concludes that the Drude weight is finite. Fig. 7 compares the numerical results for  $\sigma(q, \omega_n)$  obtained by QMC in ref. [5] to the field theory result in equation (G1). We also show the result that would be obtained by setting  $\gamma = 0$  in equation (G1), as assumed in ref. [3]. Since the agreement is good for both  $\gamma = 0$  and  $\gamma \neq 0$  taken from equation (B7), we conclude that the QMC results are not useful to decide if the relaxation rate vanishes in the integrable model. This is expected because this method cannot resolve a relaxation rate which is smaller than the separation between Matsubara frequencies,  $\omega_{n+1} - \omega_n = 2\pi T$ . Even at the Heisenberg point, where  $\gamma(T) \sim T/\ln^2(J/T)$ , the relaxation rate predicted by field theory seems to be too small to be detected by this QMC method.

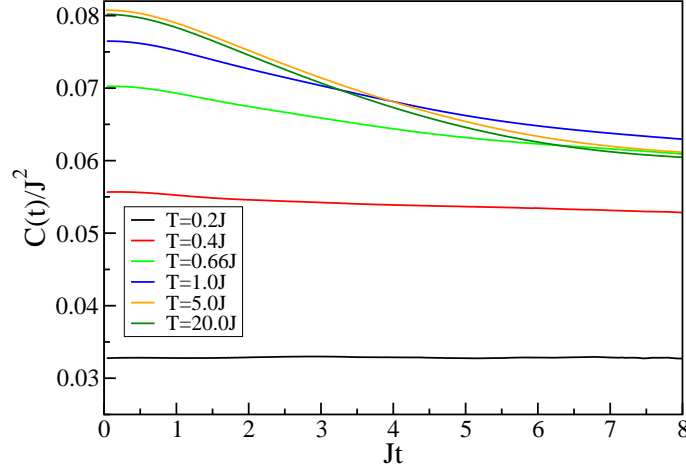


FIG. 5: Current-current correlation function  $C(t)$  for  $\Delta = 0.4$  and a magnetization  $\langle m \rangle = 0.3$ . At low temperatures the asymptotic value seems to be reached almost instantaneously. At high temperatures the data seem to be consistent with a simple exponential decay to a finite value without oscillations. Using an exponential fit and extrapolating to infinite temperature we find  $C(T \rightarrow \infty, t \rightarrow \infty) \approx 0.058$ . On the other hand, the Mazur bound, eq. (E5), yields  $2TD_{\text{Mazur}} = 0.013$ .

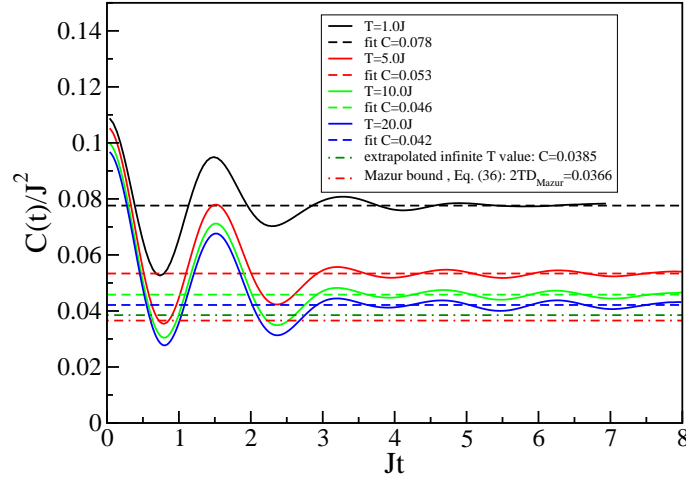


FIG. 6: Current-current correlation function  $C(t)$  for  $\Delta = 4.0$  and a magnetization  $\langle m \rangle = 0.25$ . In addition, linear fits of the data in the regime  $Jt \geq 4$  are shown. We find that the Mazur bound (E5) exhausts 95% of the Drude weight for  $T \rightarrow \infty$ .

## APPENDIX H: COMPARISON WITH BETHE ANSATZ

A finite Drude weight at finite temperatures has been obtained in two Bethe ansatz calculations.<sup>4,10</sup> Both results use the finite temperature Kohn formula<sup>1</sup> which relates the Drude weight with the curvature of energy levels with respect to a twist in the boundary conditions. Zotos<sup>4</sup> calculated the curvature by an extension of the traditional Thermodynamic Bethe ansatz (TBA) based on magnons and their bound states (strings) while Benz *et al.*<sup>10</sup> used an alternative formulation based on spinons and anti-spinons. The obtained results disagree. Problems with the approach used by Zotos have already been pointed out by Benz *et al.*. For the approach based on spinons and anti-spinons, the authors point out that “this approach is phenomenological and for the computation of the Drude weight it can not be expected to be as successful as for the free energy”. Indeed, the authors show that this approach fails at high temperatures where exact relations are violated.

In Fig. 8 we compare the Bethe ansatz results from ref. [10] at low temperatures with the Drude weight we obtain by setting  $\gamma = 0$  in Eq. (G1)

$$D(T) = \frac{Kv}{4\pi(1+b)} . \quad (\text{H1})$$

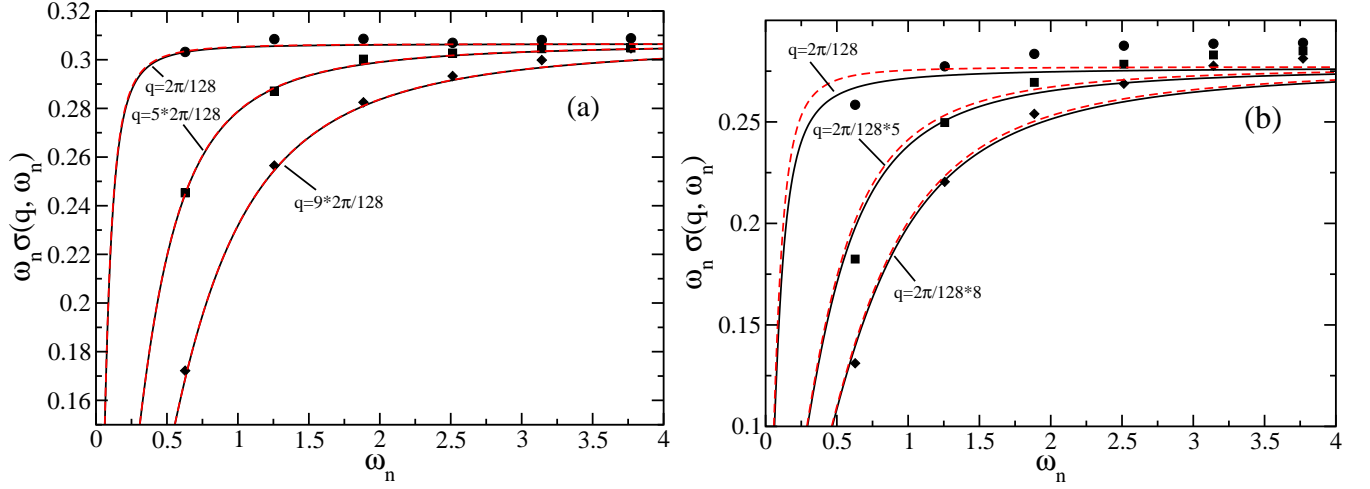


FIG. 7: QMC data (symbols) for  $T/J = 0.1$  and a system size  $L = 128$  for (a)  $\Delta = 1/2$ , and (b)  $\Delta = 1$ .<sup>38</sup> In comparison, the field theory result in equation (G1) (black solid lines) and the result obtained by setting  $\gamma = 0$  (red dashed lines) is shown. The agreement is good, in particular, for  $\Delta = 1/2$ . In this case it is clearly impossible to decide whether or not the Drude weight is finite based on the QMC data. For  $\Delta = 1$  the effect of  $\gamma$  is largest, however, here also the finite size corrections are large so that it seems again practically impossible to detect a finite Drude weight by QMC.

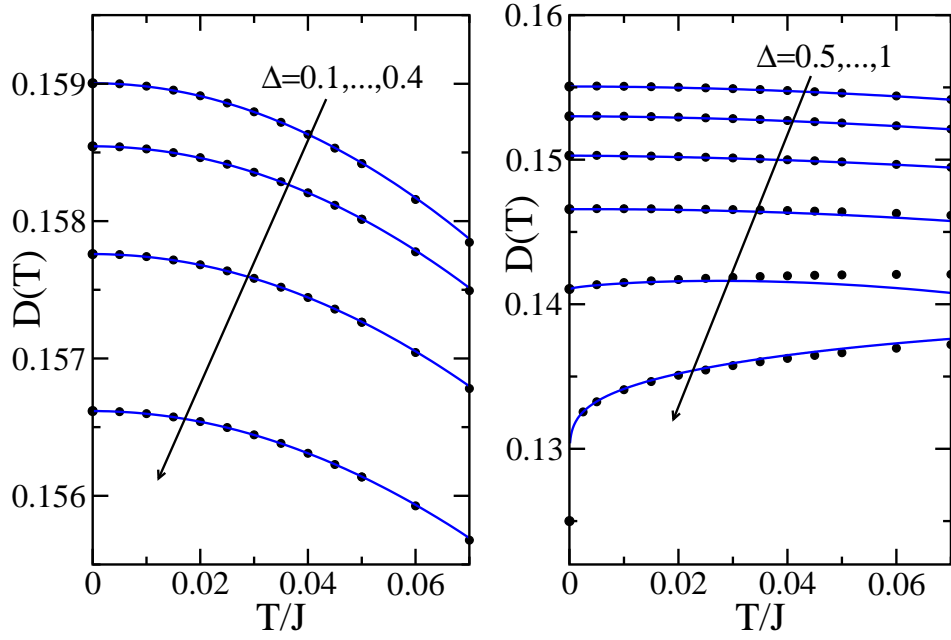


FIG. 8: The Bethe ansatz results from ref. [10] (dots) compared to the field theory formula (H1) (lines) obtained by setting  $\gamma = 0$  in Eq. (G1) by hand.

The agreement is excellent. This Bethe ansatz calculation apparently does get the temperature dependent parameter  $b$  right while, on the other hand, completely missing the decay rate  $\gamma$ . We want to stress again that our numerical results for  $C(t)/2JT$  shown in Fig. 3(c) are already smaller than  $D(T)$  obtained this way, proving that  $\gamma$  is nonzero.

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